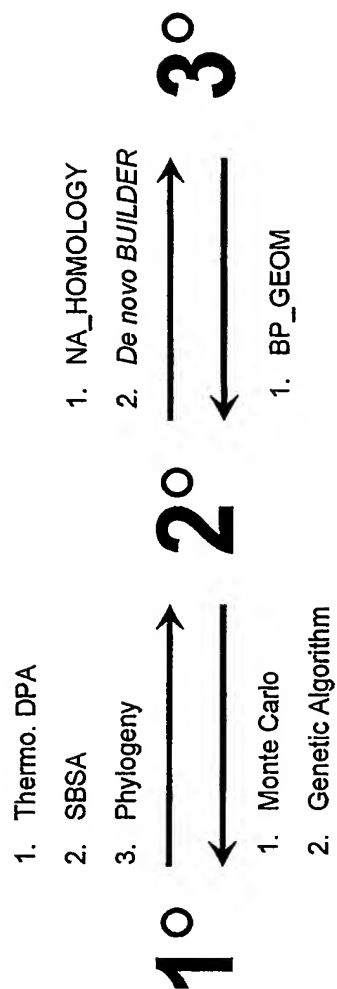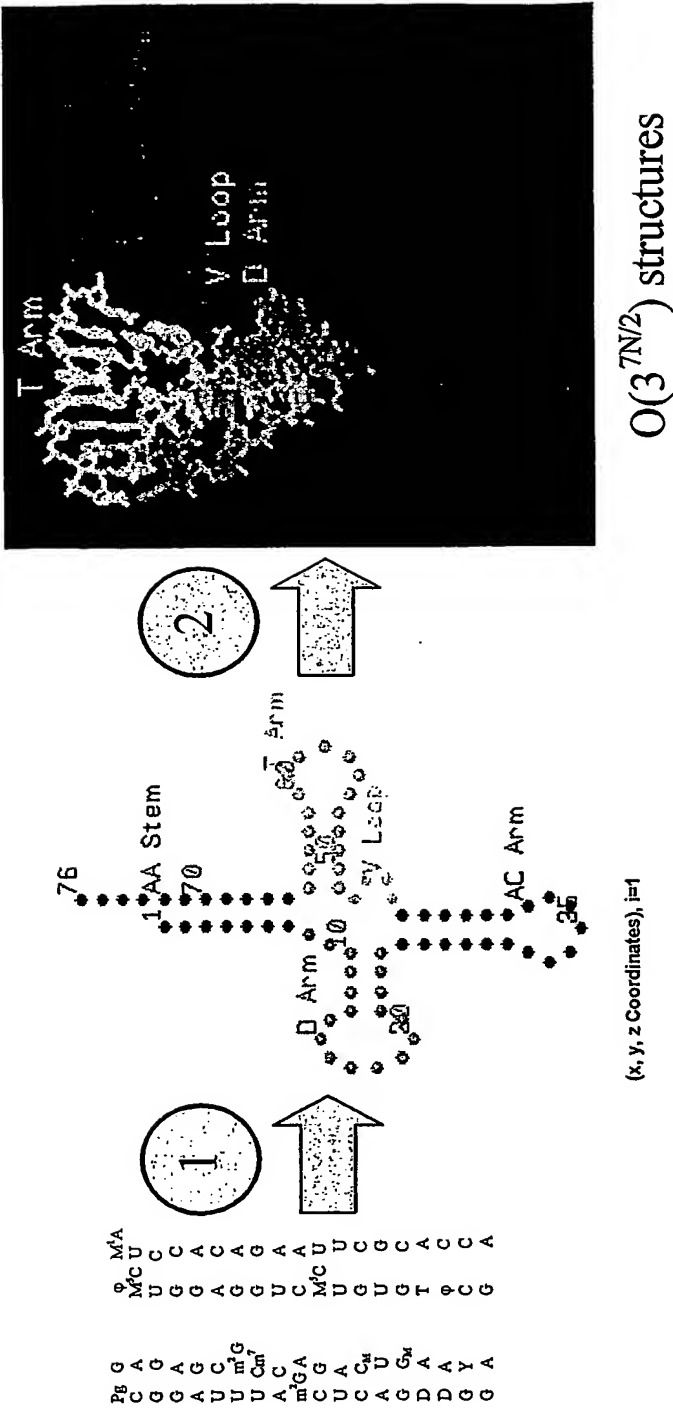FIGURE 1

FIGURE 2

FIGURE 3

Homology Modeling

Input File Window

C:\Documents and Settings\John SantaLucia\Desktop\5S project 5-1-04\1JJ2_5S added bases 5-25-04 2.PDB   BROWSE...

Load information from input file   122 residues were found in input file !

Alignment window

UUAGGCGGCCACAGCGGUGGGGUUGCCUCCCGUACCCAUCCCGAACACGGAAGAUAAGCCCACC

v v v v v   COPY BELOW   v v v v v

Load new sequence from the file   SBSA   Update Substitution List

Substitution Window -- ['All Data is CASE Sensitive]

Residues from input for: New Residues: Chain: UPDATE LIST

Chain: 9

U	1
U	2
A	3
G	4
G	5
C	6
G	7
G	8
C	9
C	10
A	11

Delete selected

122 residues were found for this chain!   Load from a file ...

Options

☑ Add hydrogens
☐ Print initial energy
☐ Print final energy
☐ Close deletion gaps
☐ Close insertion gaps
☐ Optimize with Powell
☐ DSTA on substituted
☑ DSTA on all residues
☐ DSTA on positive ens
☐ Leave only P atoms
☐ Remove Bases

RUN !

Only for testing

Counter 0

Gap Size (RMSD) 0

Compute, Print H-bonds

RMSD

Message Window

Performing Chi Dihedral optimization for missing bases... Done!

Ouput File Window

C:\Documents and Settings\John SantaLucia\Desktop\5S project 5-1-04\1JJ2_5S added bases 5-25-04 2.PDB   BROWSE...
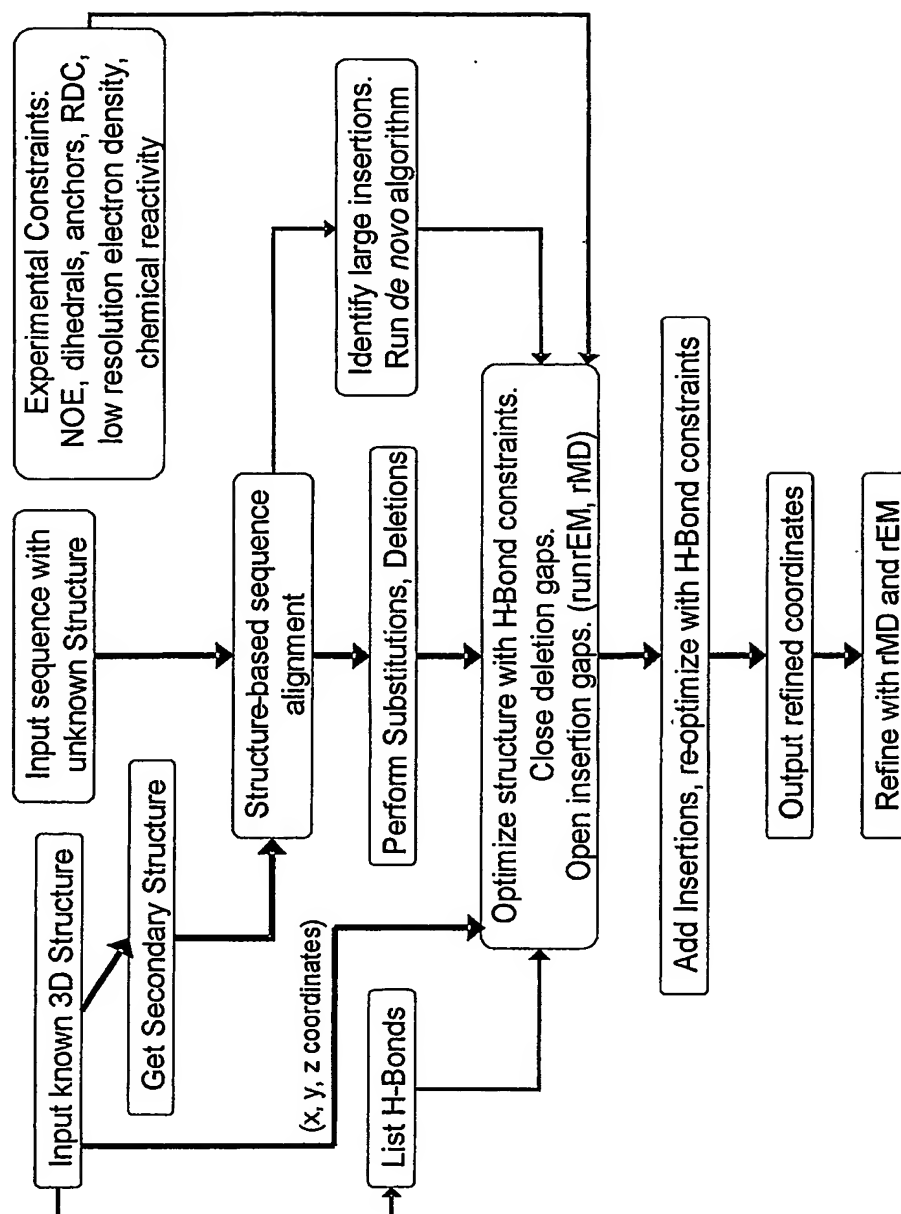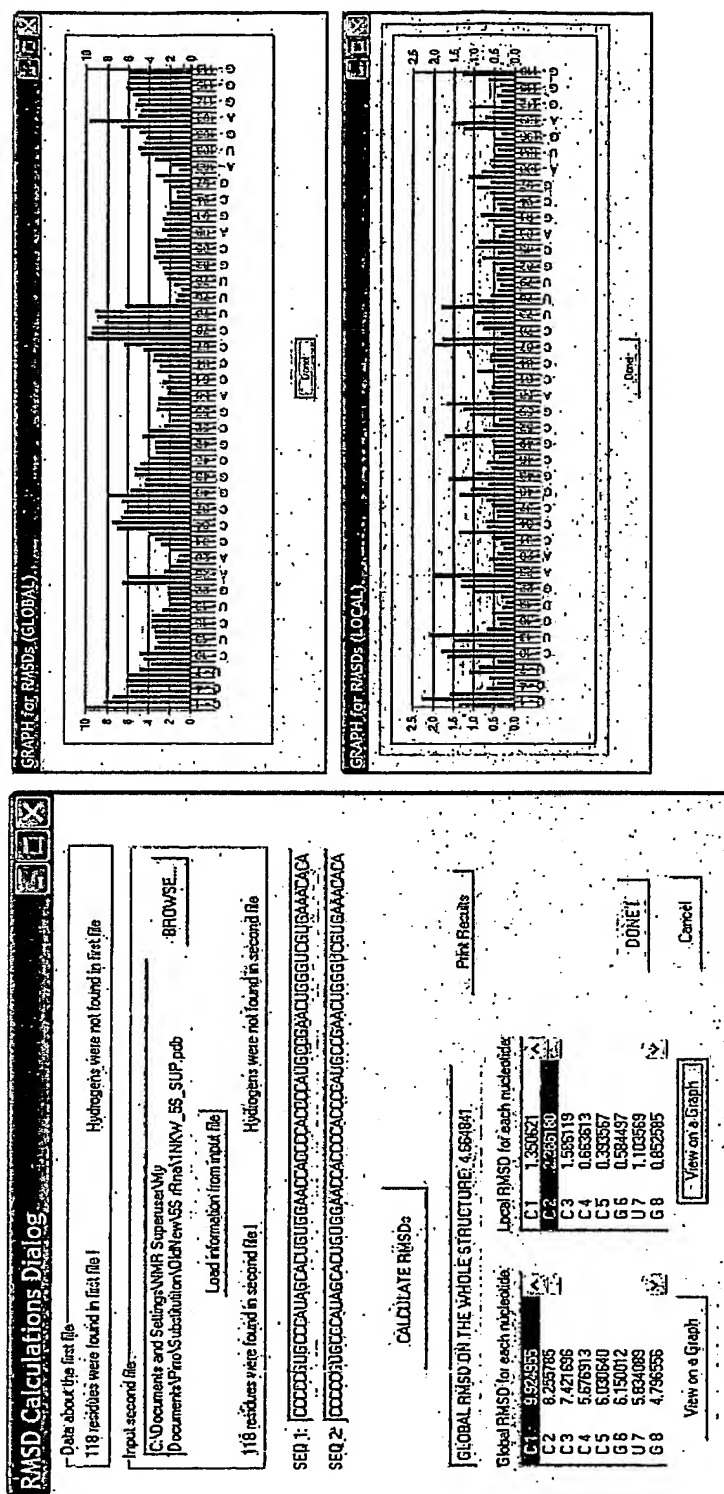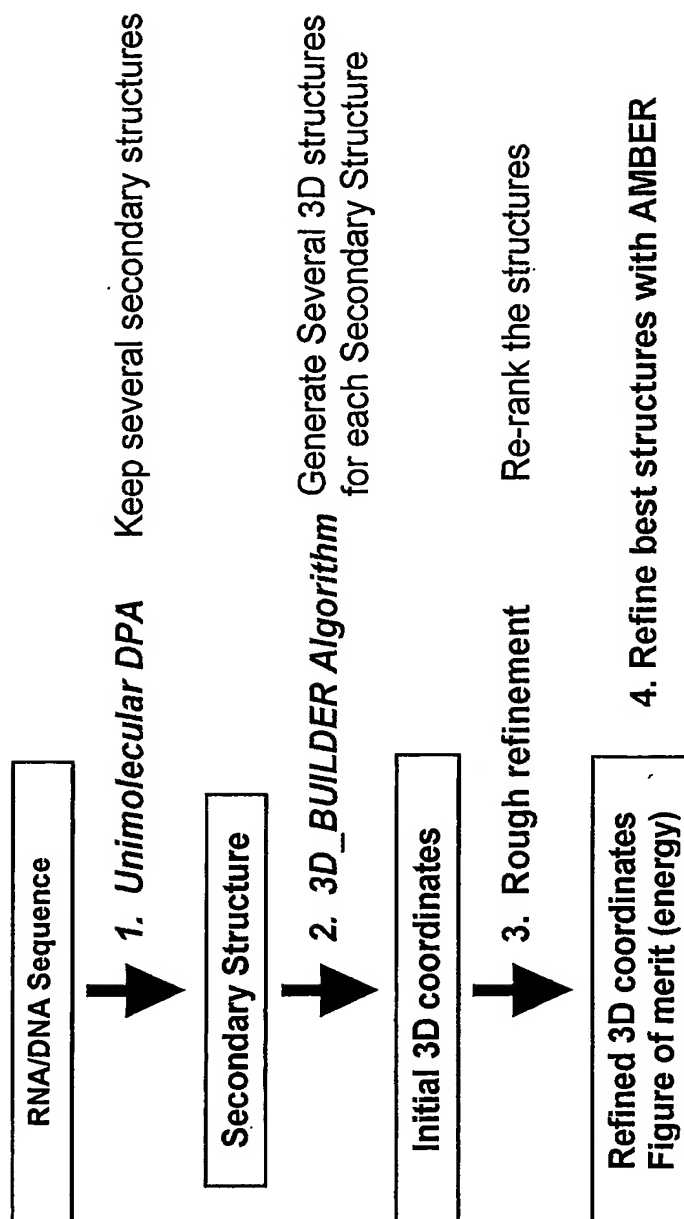
Save data in output file   END PROGRAM

FIGURE 4

FIGURE 5

FIGURE 6

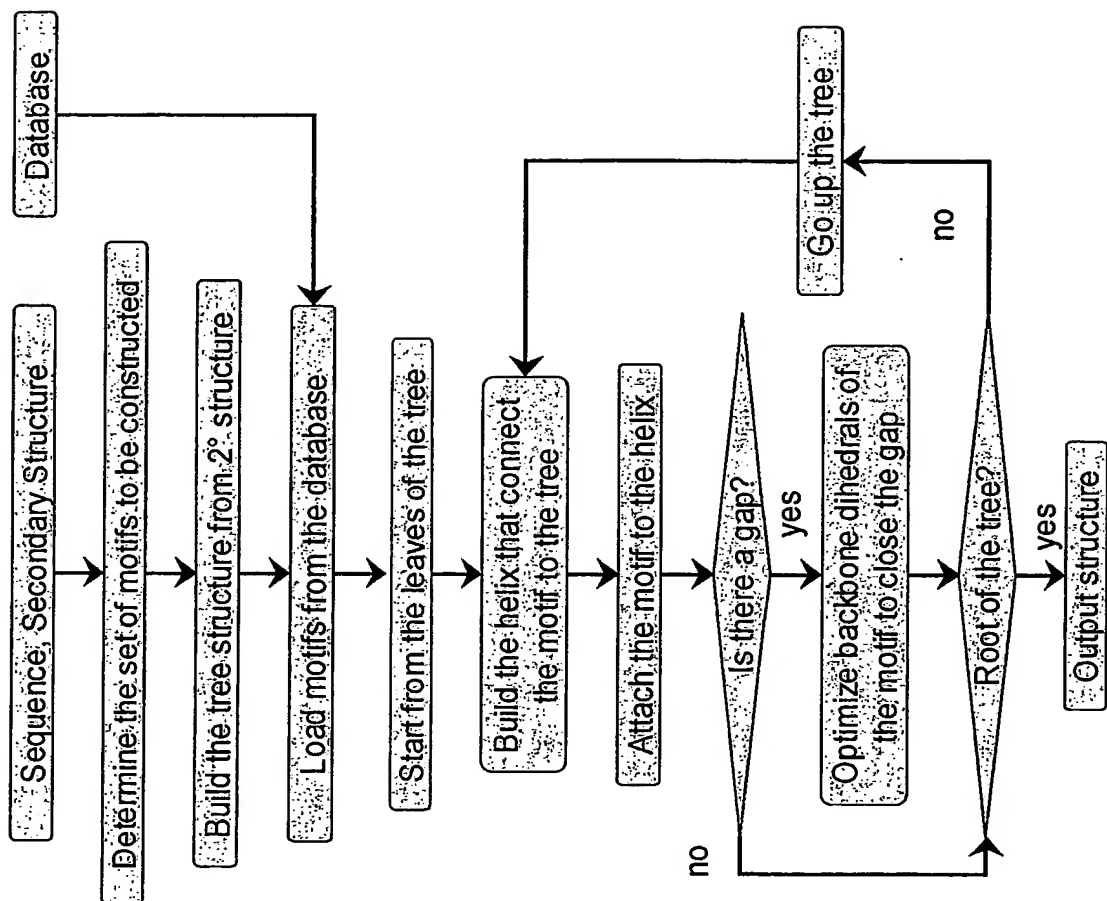FIGURE 7

FIGURE 8

FIGURE 9

X-ray: 1EHZ

After DSTA
Optimization
RMSD = 1.46

After 3 substitutions
and deletion
RMSD = 2.05 Å

FIGURE 10

NMR: 1FHK

After DSTA Optimization RMSD = 1.35

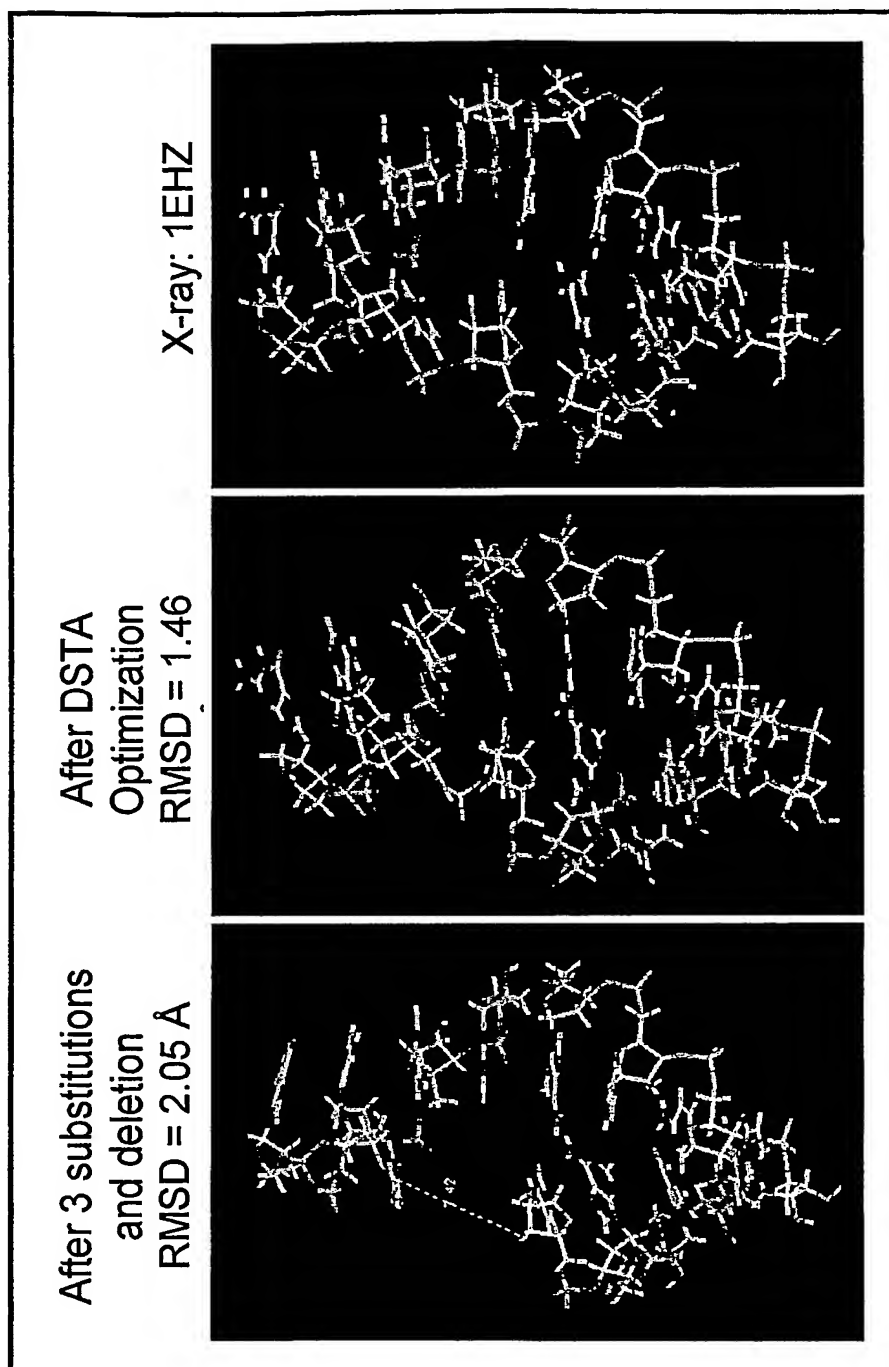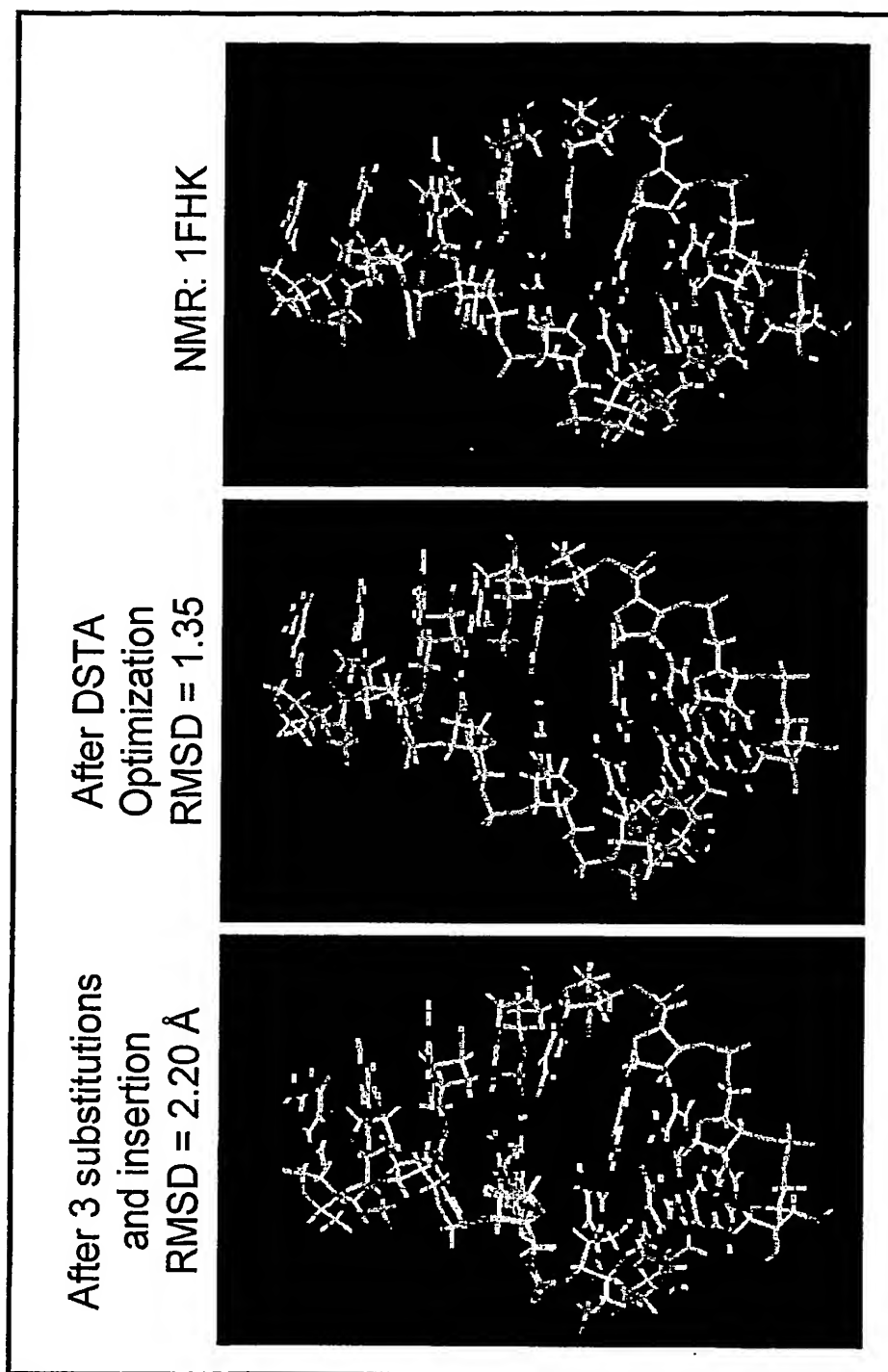After 3 substitutions and insertion RMSD = 2.20 Å
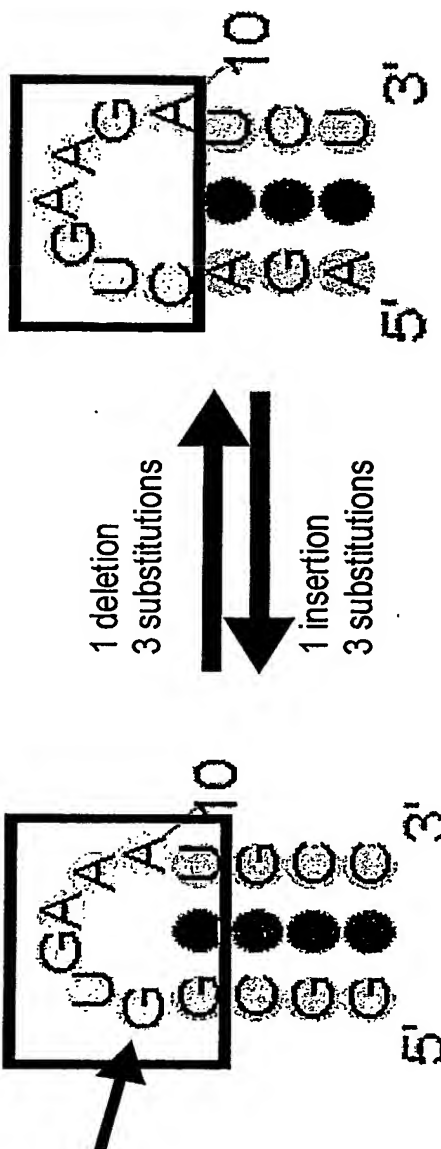
FIGURE 11

```
Motif type:    Hairpin
Motif size:    3
Sequences:     CUCAG, CUAAG
Source:        1NKW
Positions 331-333
Resolution:    3.0
ATOM  6145  P    C  0  330   -42.207  137.234  85.023  1.00  48.85  P
ATOM  6146  O1P  C  0  330   -43.221  138.159  84.459  1.00  48.85  O
ATOM  6147  O2P  C  0  330   -41.551  136.236  84.137  1.00  48.85  O
ATOM  6148  O5*  C  0  330   -41.069  138.098  85.722  1.00  48.85  O
ATOM  6149  C5*  C  0  330   -41.357  138.842  86.901  1.00  48.85  C
ATOM  6150  C4*  C  0  330   -40.085  139.347  87.534  1.00  48.85  C
ATOM  6151  O4*  C  0  330   -39.275  138.237  88.009  1.00  48.85  O
ATOM  6152  C3*  C  0  330   -39.142  140.097  86.615  1.00  48.85  C
ATOM  6153  O3*  C  0  330   -39.580  141.430  86.387  1.00  48.85  O
ATOM  6154  C2*  C  0  330   -37.842  140.026  87.402  1.00  48.85  C
ATOM  6155  O2*  C  0  330   -37.815  140.934  88.486  1.00  48.85  O
ATOM  6156  C1*  C  0  330   -37.898  138.592  87.935  1.00  48.85  C
Chi DIHEDRAL = -3.10169 radians
C4'-O4'-C1'-N9 DIHEDRAL = -2.11876 radians
O4'-C1'-N9 bond angle = 1.90932 radians
```

FIGURE 12

FIGURE 13
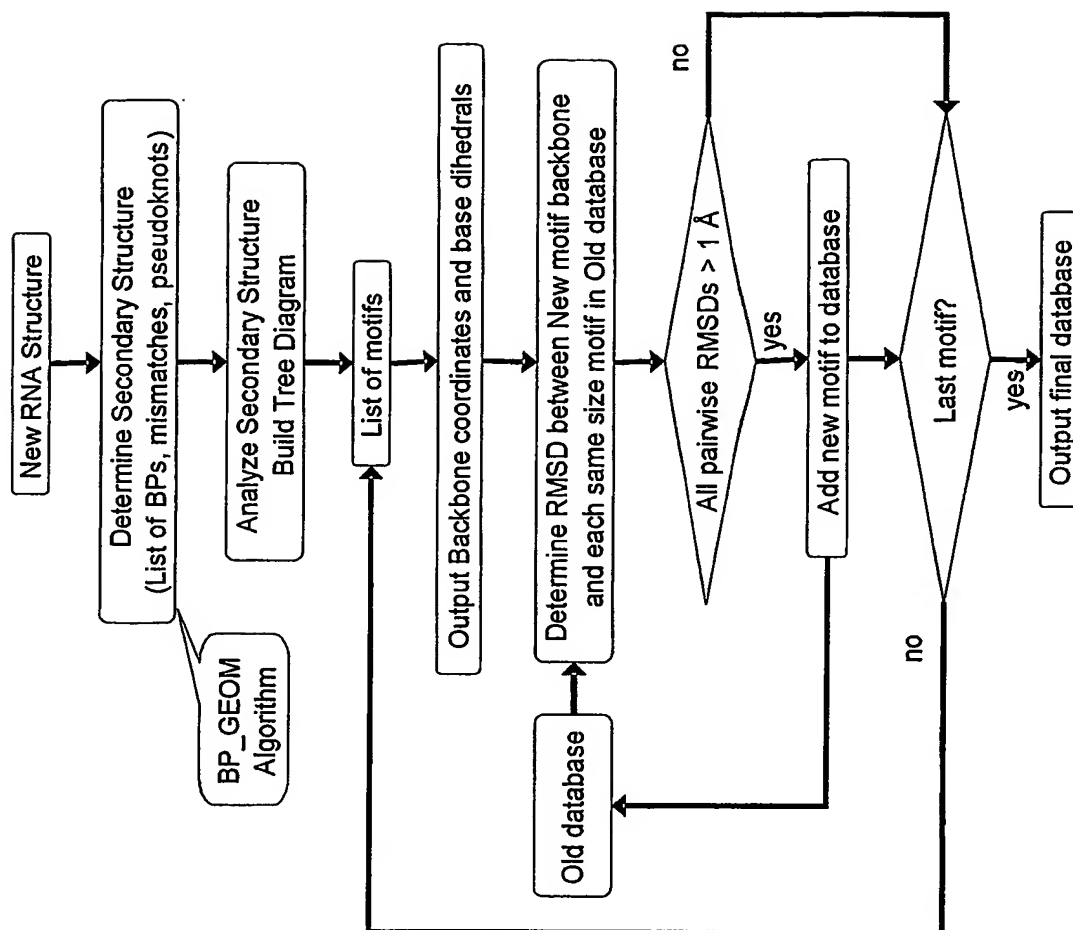
Table 1: Structured Motif Database									
Hairpins[a,b,c,d,e]		Bulges[b,c,d,e]		Internal Loops[b,c,d,e]		Internal Loops[b,c,d,e]		Multiloops	
Length	Number	Length	Number	Length	Number	Length	Number	stems	Number
3	6	1	31	1x1	42	3x9	1	3	55
4	64	2	15	1x2	18	4x4	6	4	28
5	23	3	1	1x3	12	4x5	15	5	11
6	20	4	0	1x4	8	4x6	3	6	4
7	26	5	0	1x5	1	4x7	3	7	2
8	23	6	2	2x2	13	5x5	6	11	1
9	16	7	0	2x3	15	5x6	12		
10	11	8	0	2x4	7	5x7	7		
11	8	9	1	2x5	2	5x8	5		
12	6			2x6	2	6x6	4		
13	4			2x7	1	6x7	4		
14	0			3x3	17	7x7	3		
15	5			3x4	11	other	24		
19	1			3x5	5				
				3x6	4				
				3x7	5				

References for crystal structures
a 1EHZ tRNAphe
b 1HR2 group I intron
c 1J5E 16S rRNA *Thermus thermophilus*
d 1JJ2 23S rRNA *Haloarcula marismortui*
e 1NKW 23S rRNA *Deinococcus Radiodurans*

FIGURE 14

CLUSTAL-W sequence alignment of 5S rRNA

Score = 68/129 = 52.7%   Correct alignment = 100/129 = 77.5%

```
1JJ2  ----UUAGGCGGCCACAGCGGUGGGGUUGCCUCCGUACCCAUCCGAACACGGAAGAUAAG
1NKW  ACACCCCCGUGCCCAUAGCACUGUGA-ACCACCCCACCCCAUGCCGAACUGGGUCGUGAAA
      * * *** ***    ** ** *** ****** ******  *  *  **
```

```
1JJ2  CCCACCAGCGUUCCGGGGAGUACUGGAGUGCGCGAGCCUCUGGGAAACCCGGUU--CGCCGCCACC-
1NKW  CACAGCAGCG--CCAAUGA-UACUCGGAC-CGCAGGGUCCCGGAAAAAGUCGGUCAGCGCGGGGGUUU
      * ** ****** **  ** ***** *     *** * ** *** **** ***  *
```

SBSA Alignment of 5S rRNA

IDENT = 65/129 = 50.4%   Correct alignment = 129/129 = 100%

```
       ddd   LLLLLLL  d   LLLLLLLL  i  mLLLLLLL          RRRR  RRm
1JJ2  ---UUAGGCGGCC-ACAGCGGUGGGGUUGCCUCCGUACCCAUCCGAACACGGAAGAUAAG
1NKW  ACACCCCCGUGCCCAUAGCACUGUGA-ACCACCCCACCCCAUGCCGAACUGGGUCGUGAAA
       LLLLLLLLLLi i  LLmLLLLL  d  LLLLLLL           RRRR  RRR
IDENT  --    *** *-****- ** **  -** ***    ****** ******* ** * **-
```

```
       RRRRRR RR mmLLLLL  i  LLLLLLLL    RRRRRRRR         RRRRRmm RRRRRR       ddd
1JJ2  CCCACCAGCGUUCCGGGGAGUACUGGAGUGCGCGAGCCUCUGGGAAACCCGGUUCGCCGCCACC---
1NKW  CACAGCAGCG--CCAAUGA-UACUCGGA-CCGCAGGGUCCCGGAAAAAGUCGGUCAGCGCGGGGGUUU
       RRRRRm RR ddLLmLL  d  LLmLLLdLL    RRRRRmRR    RRmRR    RRRRRRRRRRRii
IDENT  * ** ****** **--  ** **** *--  ***--*  **---*--*-**-***  -*****-  **     -
```
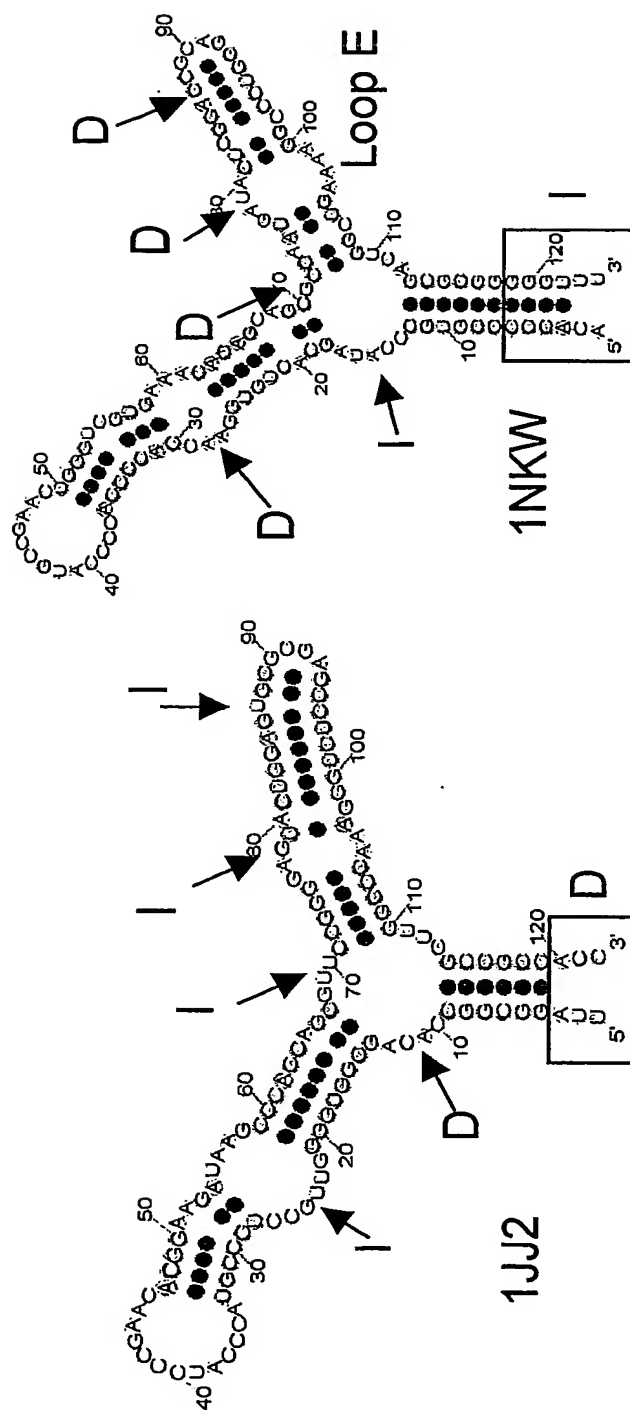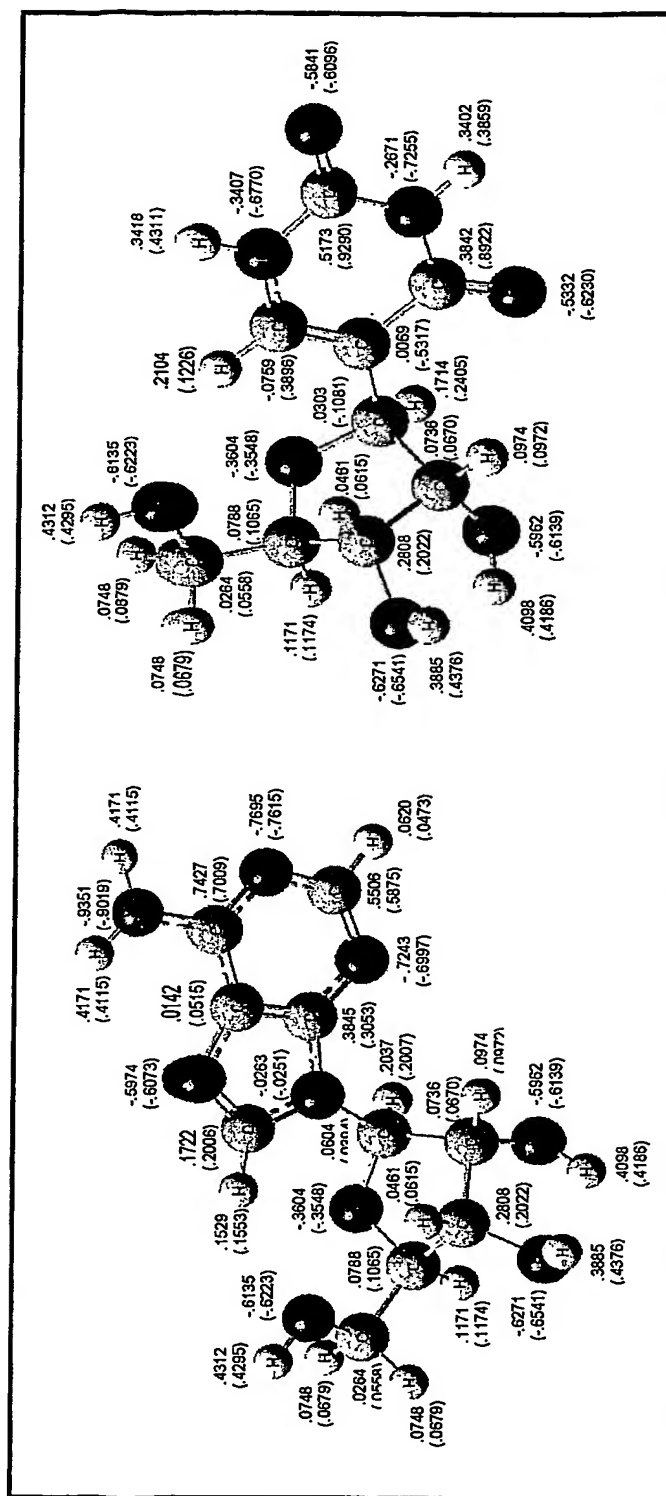
FIGURE 15

FIGURE 16

FIGURE 17

FIGURE 18

FIGURE 19

- N=Number of Nucleotides
- IPD= Inter planar distance
- Dist= Distance

Start

Read Input Structure (x, y, z Coordinates), i=1

i < N?
yes / no

i = i+4

j < N ?
yes / no

GC or UA ?
yes / no

Find Mismatch type

i=i+1

if Dist <3.5 & IPD < 2.0
yes

i, j forms Base pair

i=i-1

List of Base Pairs.

Find Chord crossings

Update BP list

If Chord Crossings > 0
yes / no

Find BP that crosses max number of chords. ADD to PK list. Delete the Chord.

END